Beam Dynamics Framework and Infrastructure

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and

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Primary contributions to the work in this talk come from

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Lawrence Berkeley Lab: *Ji Qiang and R. R.*

Tech-X: *John Cary, Douglas Dechow, Stefan Muszala, Seith Veitzer*

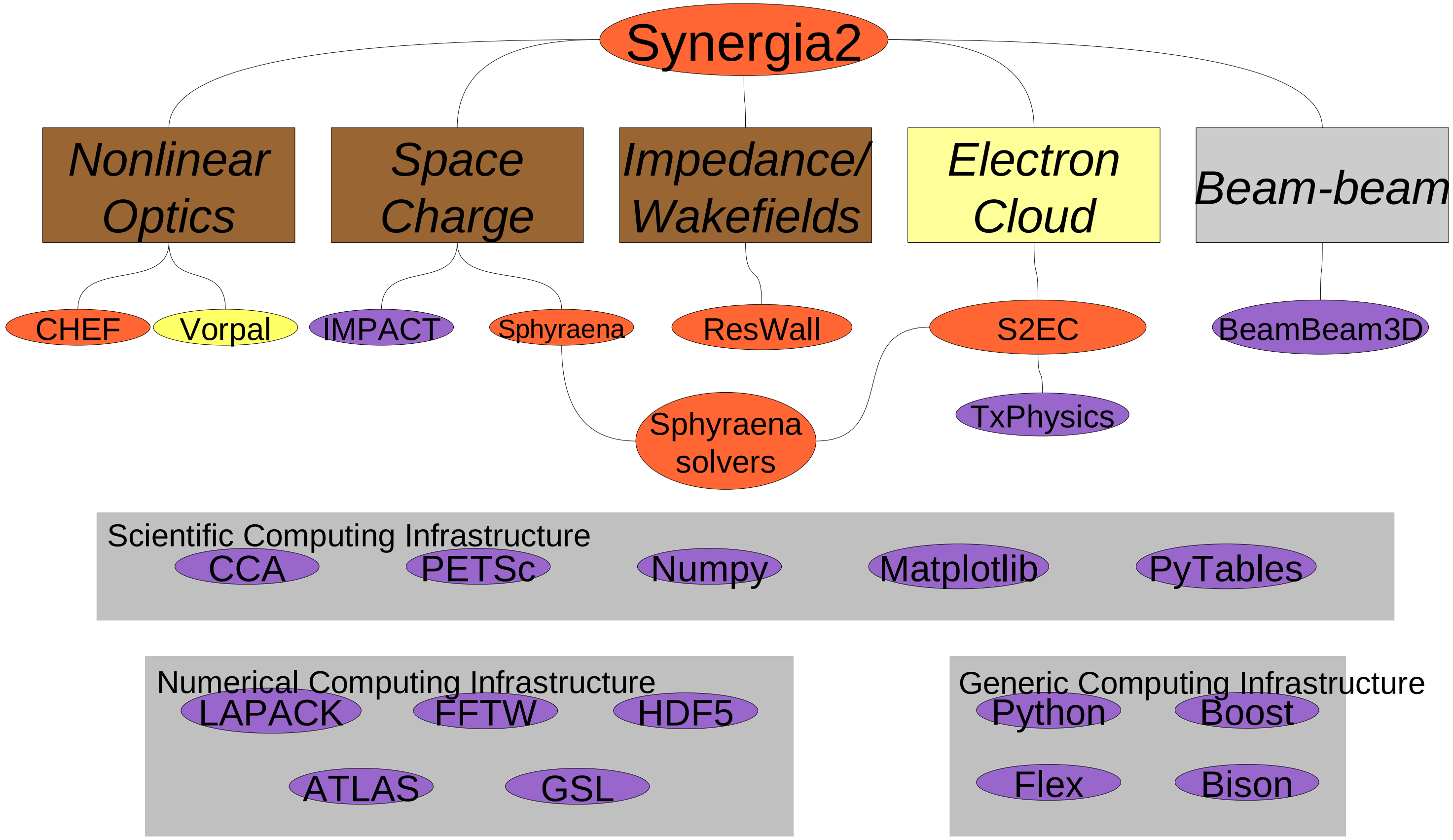
SciDAC Math/CS Collaborators: TASCS, PERI, TOPS

Overview

- Introduction
- Infrastructure
- Porting
- Solver development
- Performance and scaling
- Beam dynamics capability development
- Applications

Introduction

- Accelerator physics frameworks are a way to combine physics capabilities

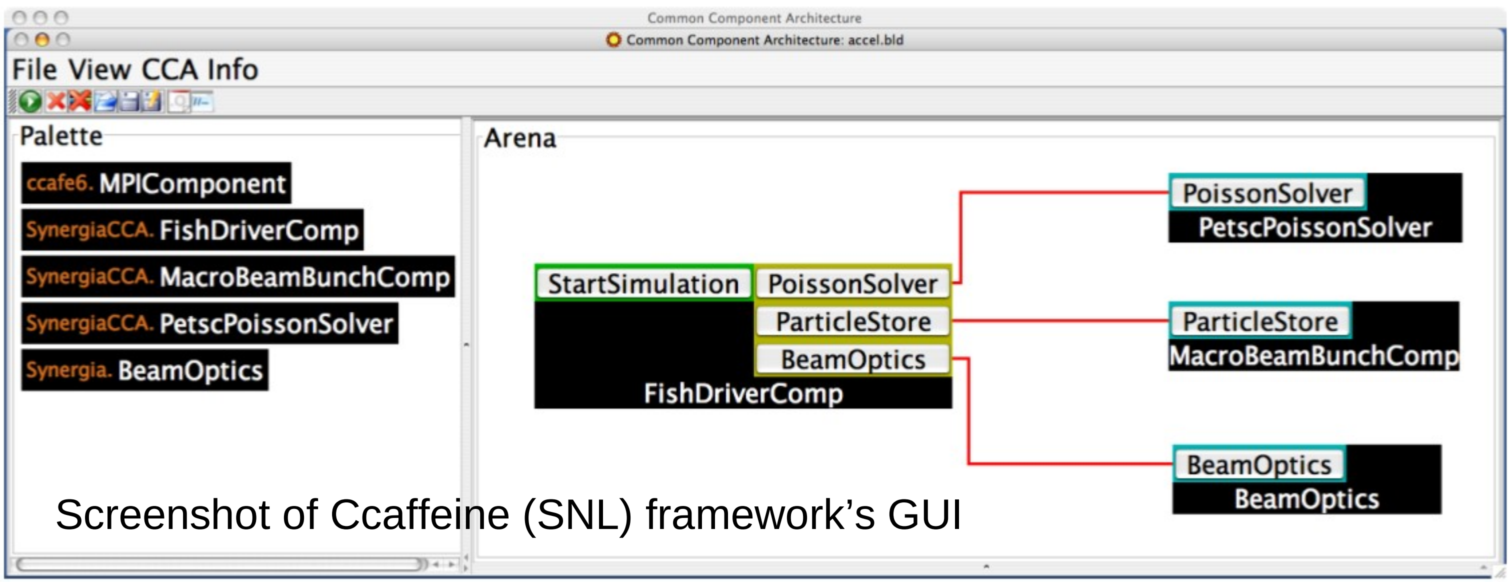


Component motivation

- Complexity of scientific software increases with simulation fidelity, multi-physics coupling, and computer power
- Common Component Architecture (CCA) component vision: Enable the HPC community to leverage existing applications, creating modular, reusable software components that facilitate the combined use of historically independent codes to add new capabilities (see www.cca-forum.org)
- Approach: Develop a prototype accelerator simulation from existing codes that were not originally designed to work together; leverage external math/cs tools developed by experts (TOPS/PERI)
- Long-term Goal: Foster a component community in computational accelerator physics, with emphasis on easily incorporating new algorithms and performance enhancements

Infrastructure: components prototype toolkit

- **Components:** interact only through well-defined interfaces
- **Ports:** interfaces through which components interact (*provides/uses* pattern)
- **Framework:** holds components while applications are assembled and executed, controls the connection of ports, provides services to components



Screenshot of Ccaffeine (SNL) framework's GUI

- **Key features of CCA components**
  - Programming language interoperability
    - Via SIDL/Babel (LLNL)
  - Dynamic composability
  - Encouragement of common interfaces

- **Sample simulations**
  - FODO cell demo
  - Apply space charge kick
  - Code at pcac.fnal.gov

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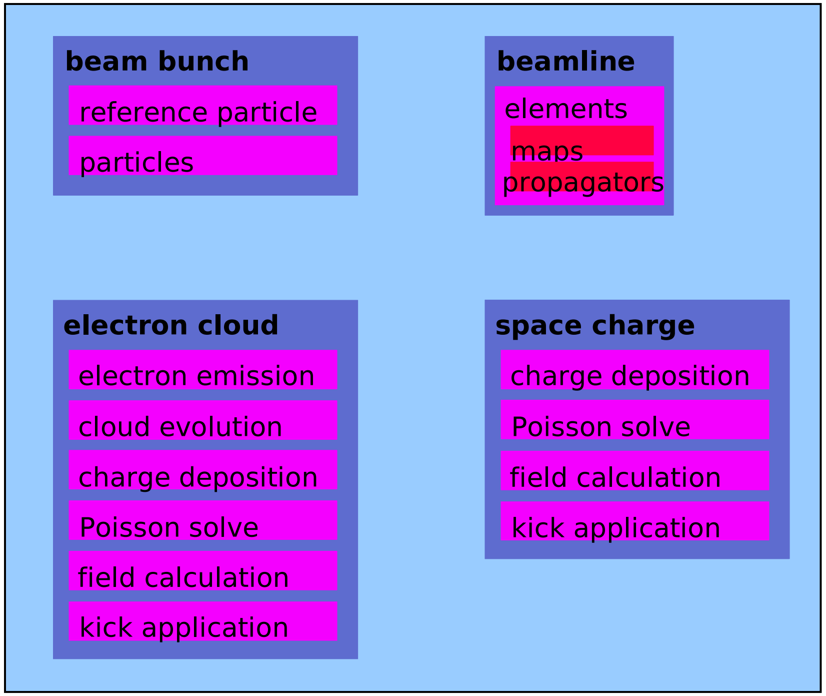
Infrastructure: components defining interfaces

- **Refactoring Synergia2 and exploring interface issues for common functionalities**
  - Beam bunch
  - Beamline
    - Demonstrated interchanging CHEF and MaryLie beamline components at the map level, even though beamline models themselves are very different
  - Space charge
    - Synergia2 can use space charge modules from either IMPACT or Sphraena
  - Electron cloud
- **Challenges**
  - **Granularity:** Overheads that apply *per particle* get an extra factor of ~10^7
    - unacceptable … use aggregation
  - **Parallel decomposition** of fields, etc., must be compatible: may force coarser granularity



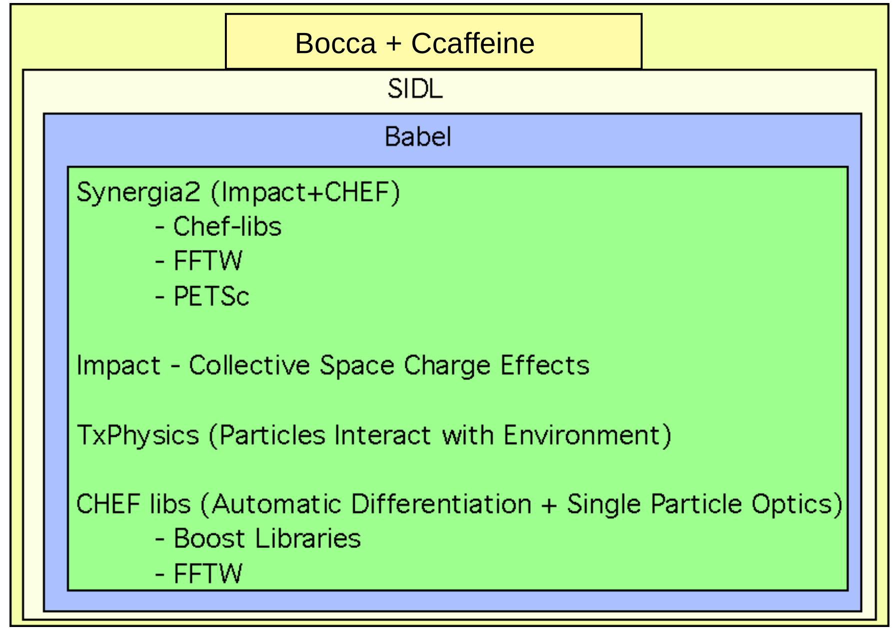
References: *Multiscale, Multiphysics Beam Dynamics Framework Design and Applications,* J. Amundson, D. Dechow, L. McInnes, B. Norris, P. Spentzouris and P. Stoltz, J. Phys.: Conf. Ser. 125 (2008) 012001.

Common Component Architecture for Particle Accelerator Simulations, D. Dechow, B. Norris, and J. Amundson, Proceedings of HPC-GECO/CompFrame'07, October 21-22, 2007, Montreal, Quebec, Canada, ACM, 2007.

Infrastructure: components CCA electron cloud

Beam Dynamics Toolkit

- F90-based beam **optics components** (quadrupoles and drifts) from the MaryLie/Impact application (LBNL)
- C++ and F90 **particle store components** from the Synergia2 framework (FNAL)
- A newly implemented C++-based **space charge solver**, Sphyraena, which uses Synergia2, PETSc (ANL), and FFTW
- C++ **ionization components** from TxPhysics (Tech-X)



Uses CCA tools:

- **Bocca**: Creates skeletal structure for a component and its interfaces, including the entire build system
    - ComPASS provided feedback to Bocca developers on new functionality needed
- **SIDL/Babel:** Provides language interoperability

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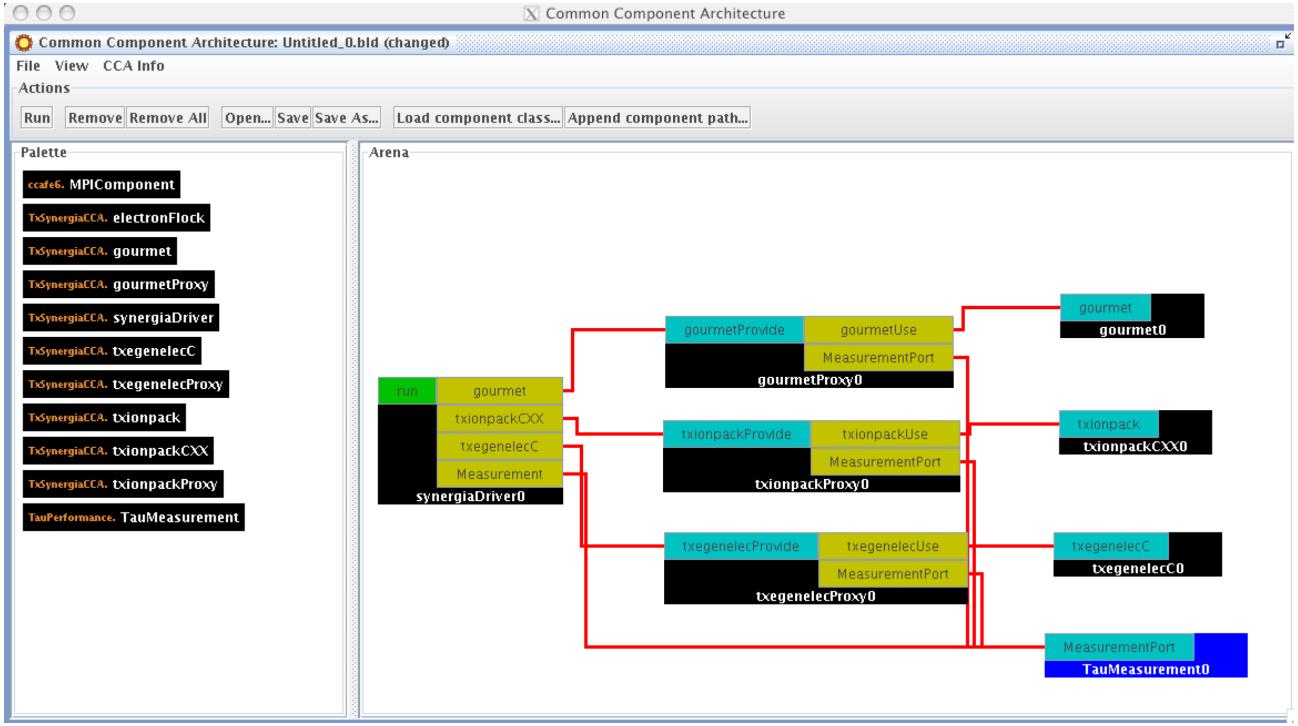
Infrastructure: components CCA ecloud performance evaluation



- Validated performance of component and non-component codes
- Using automated performance proxy generation facilities available to all CCA components (via TAU, Univ. of Oregon, affiliated with PERI)
- Time for solvers and integrators dominates; ongoing work with TOPS to address solvers issues

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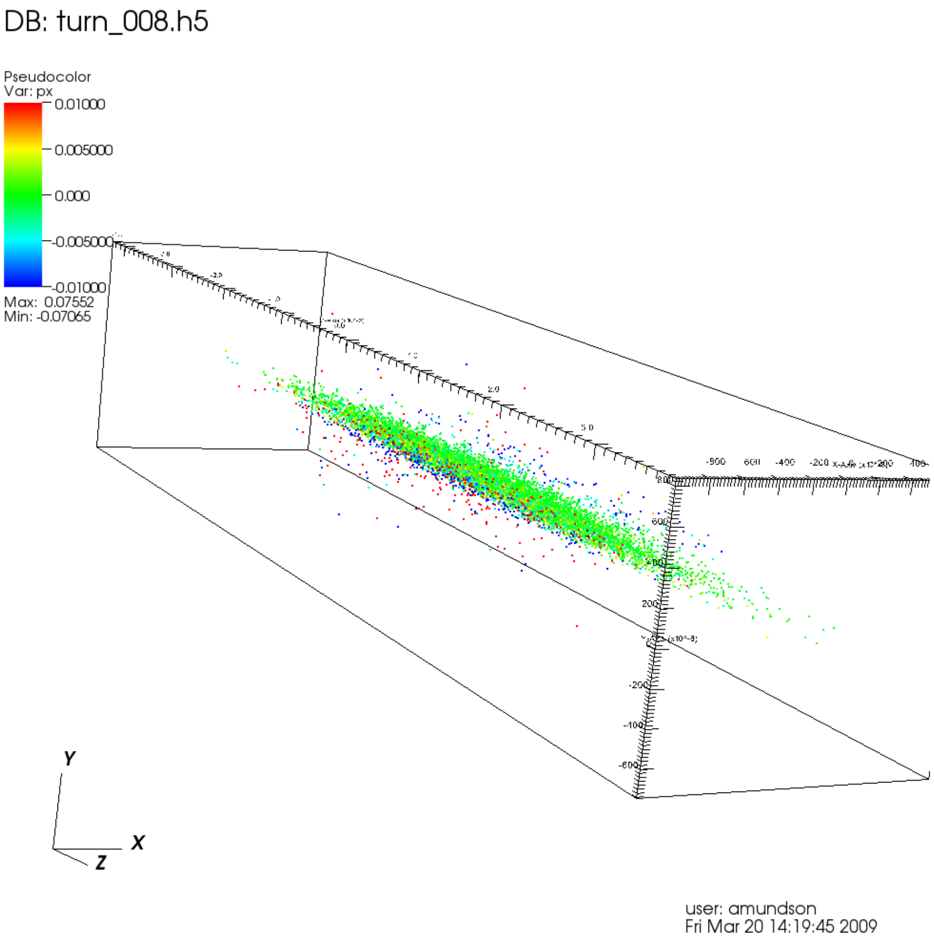
Infrastructure: components ongoing and future work

- Immediate priorities: Critical for ComPASS component integration
  - Collaborating with TASCS to address
    - Babel/SIDL interlanguage capabilities with struct support, broad support of Fortran compilers
    - Ability to run on leadership class facilities (including Cray XT4, BG/P)
  - Define new space charge interface (interchangeable use of several space charge algorithms)
  - Evaluate performance of original Synergia application and component variant on space charge applications
- Longer-term vision: Collaborate with TASCS, PERI, and TOPS to address issues in Computational Quality of Service (CQoS) for accelerator simulations,
  - How, during runtime, can we make make sound choices for reliability, accuracy, and performance, taking into account the problem instance and computational environment?
    - Composition: select initial component implementations and configuration parameters
    - Reconfiguration: change parameters
    - Substitution: change implementations

Infrastructure: visualization

- Advanced visualization is not useful in everyday work until conversion barriers can be overcome
- Collaboration with VisIt team has produced a VisIt Synergia plugin
  - Plugin code available in Synergia repository
  - Data format standards created
  - Particle data ready
  - Field data under development



Porting: capability machines

- Porting issues are simplest for large, monolithic written in Fortran, C, or C++
- Multi-language frameworks provide more challenges
  - Synergia utilizes Python, C++, Fortran
- New machines have new complexities
  - Synergia ran on Seaborg
- Lack of shared library support on NERSC's Franklin a huge barrier
  - Porting not cost-effective at this point
- ALCF's Surveyor/Intrepid is a workable solution
  - Synergia recently ported
  - Integrating BG/P into Synergia workflow is a work in progress

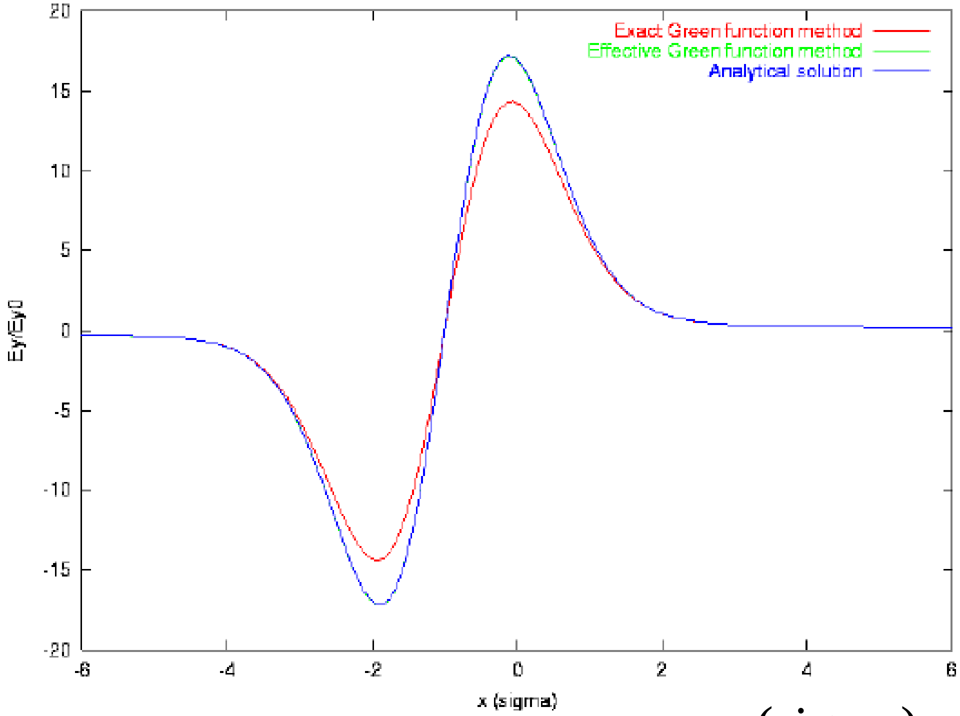
Solver development: integrated Green functions

<u>Integrated Green function Algorithm for large aspect ratio:</u>

$$\phi_c(r_i) = \sum_{i'=1}^{2N} G_i(r_i - r_{i'})\,\rho_c(r_{i'})$$

$$G_i(r, r') = \oint G_s(r, r')\,dr'$$

E_y



x (sigma)

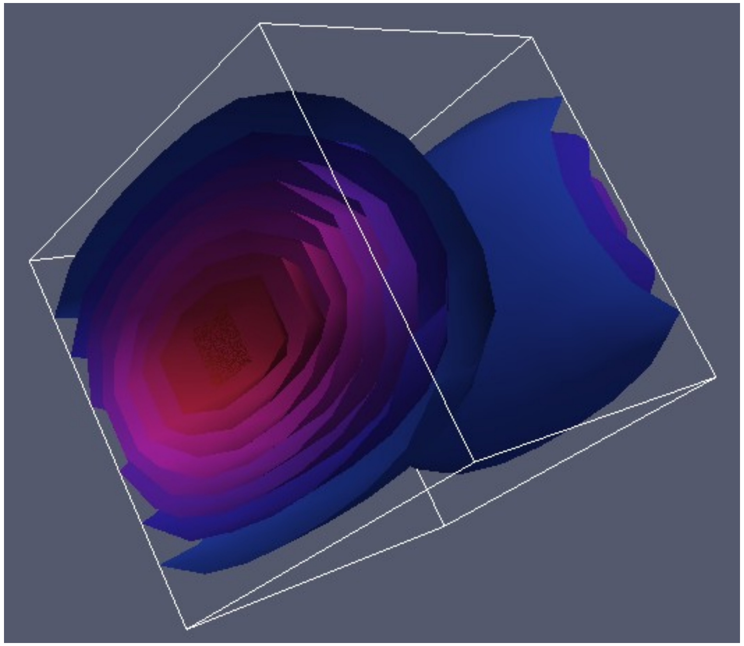
Solver development: Sphyraena

- Sphyraena is the native Synergia solver suite
  - Available for other applications
- 3D, open boundary conditions
  - FFT + Green Functions a la Hockney
    - FFTW
  - Interpolated Green Functions for high large aspect ratios
    - Optimized for z >> x,y
- 3D, closed cylindrical boundary conditions
  - FFT (z,theta), finite difference in r
    - FFTW
- 3D, closed elliptical boundary conditions
  - Finite differences, stretched grid
    - PETSc

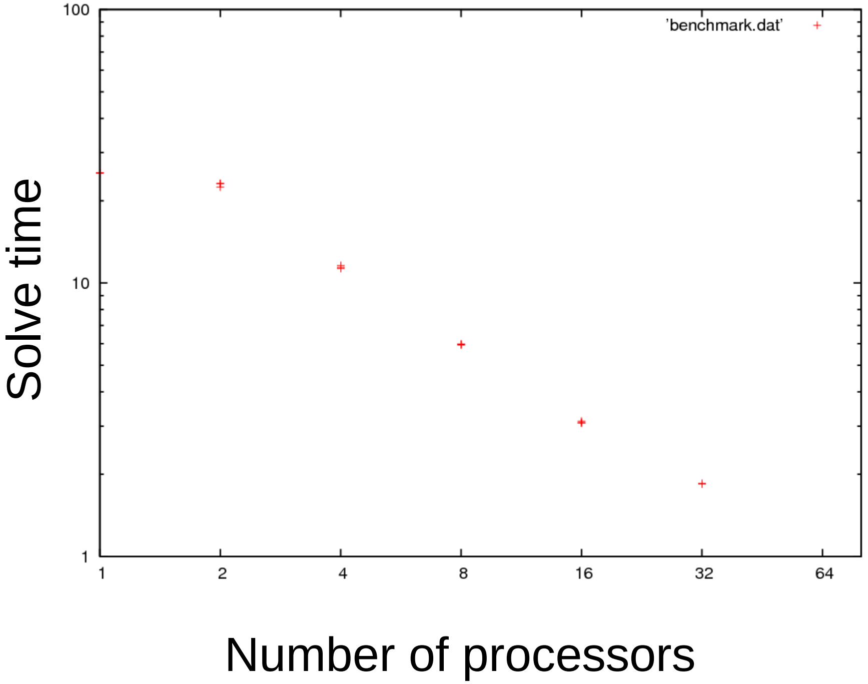
Solver development: Sphyraena elliptical solver

- New, finite-difference based elliptical solver
  - Uses PETSc

Field solution for benchmark problem



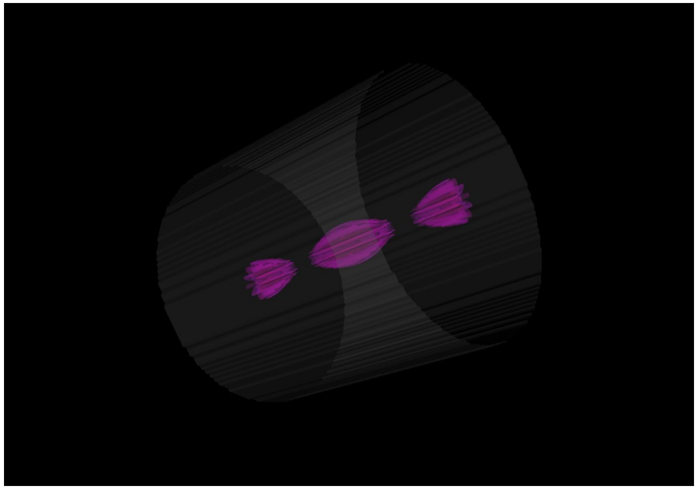
excellent parallel scaling performance provided by PETSc libraries



Solver development: testing

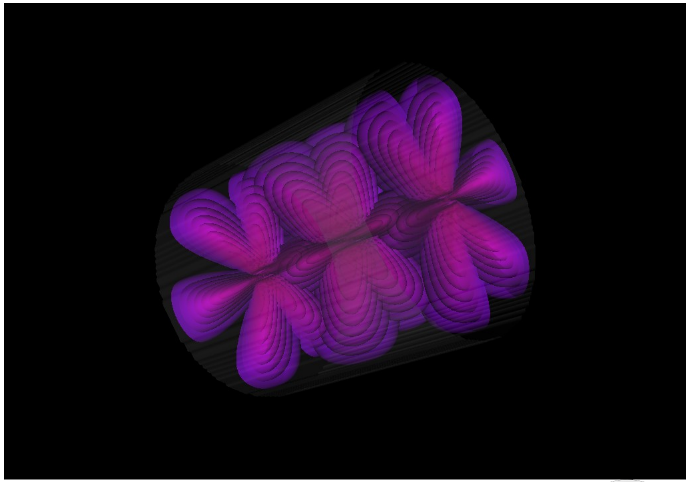
- *Full* testing of 3D solvers is not trivial
- Take a non-trivial charge density

$$\rho(r,\theta,z) = \Big[\Big(\big(18\,{r_0}^2 - 14\,r^2\big)\,\sin^2(3\,\theta) + \big(18\,r^2 - 18\,{r_0}^2\big)\,\cos^2(3\,\theta)\Big)\,\cos^2\left(\frac{\pi\,z}{z_0}\right)\,{z_0}^2 + \big(2\,\pi^2\,r^4 - 2\,\pi^2\,r^2\,{r_0}^2\big)\,\sin^2(3\,\theta)\,\sin^2\left(\frac{\pi\,z}{z_0}\right) + \big(2\,\pi^2\,r^2\,{r_0}^2 - 2\,\pi^2\,r^4\big)\,\sin^2(3\,\theta)\,\cos^2\left(\frac{\pi\,z}{z_0}\right)\Big] \Big/ \big(r^2\,{r_0}^2\,{z_0}^2\big)$$



- ... and produce a test in all coordinates

$$\phi(r,\theta,z) = \left(1 - \frac{r^2}{r_0^2}\right)\sin^2(3\theta)\cos^2\left(\pi\frac{z}{z_0}\right)$$



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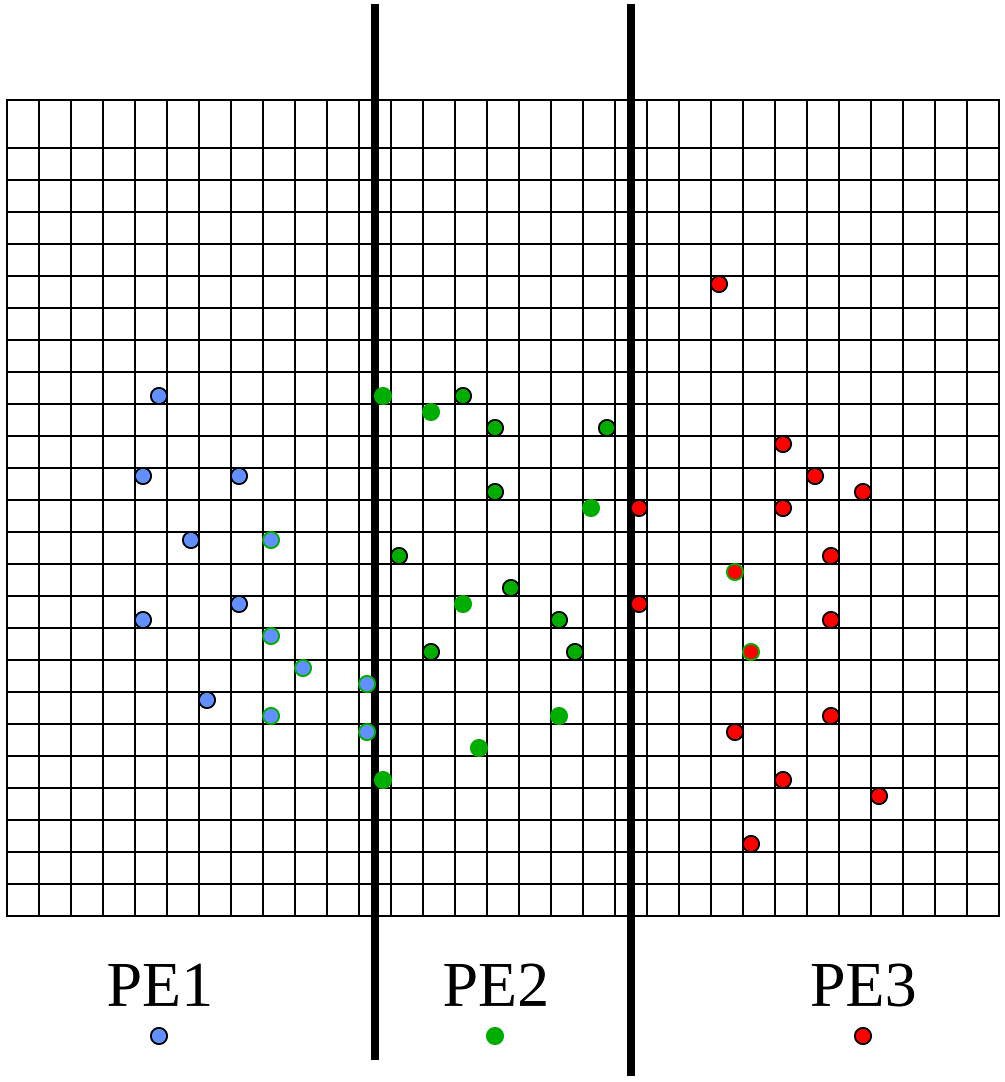
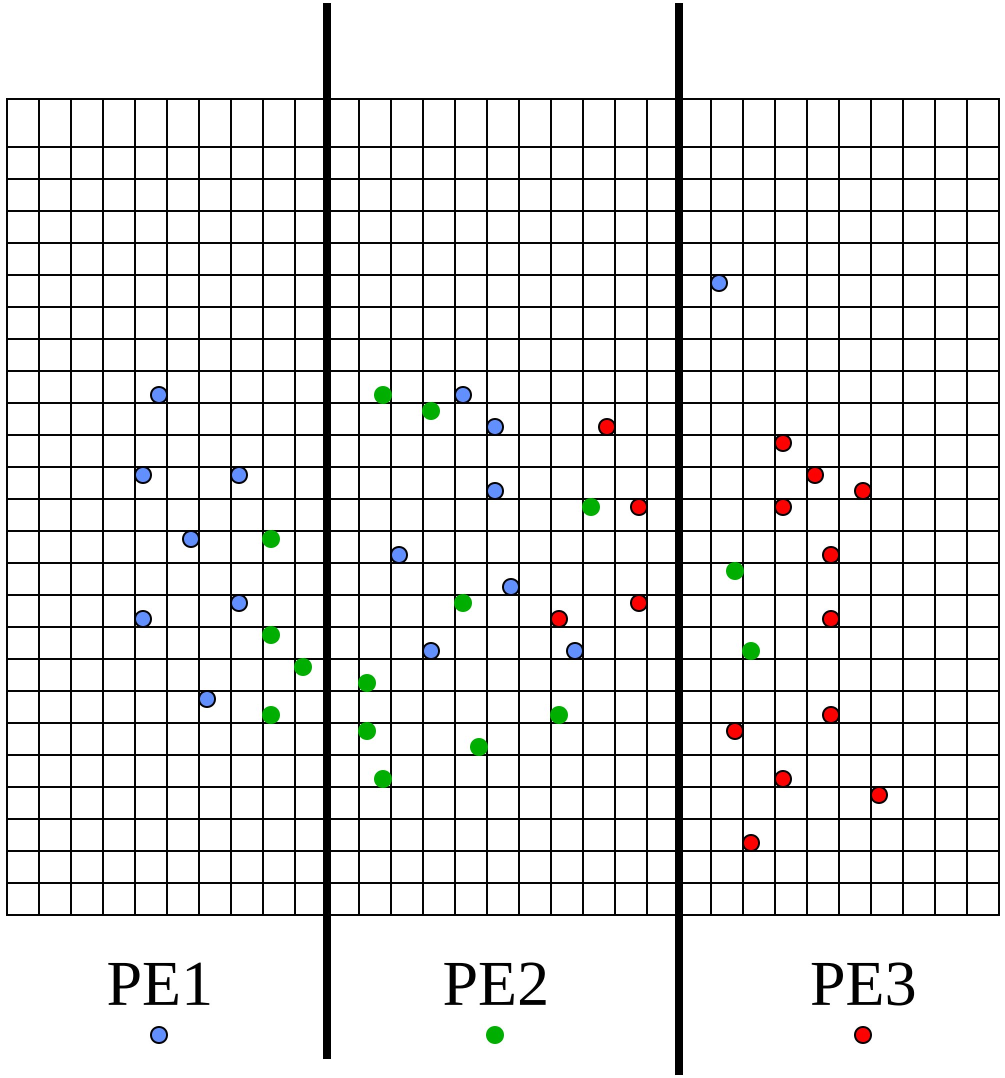
Solver development: future

- Expand boundary conditions
  - Further optimize elliptical case
- Expect to benefit from PERI optimization work
  - New postdoc
  - Collaboration with Sheri Lee has already produced substantial improvements in IMPACT
- Optimize parallelization schemes
  - Compare with other solver implementations
- Other algorithmic improvements
  - Ongoing research

Scaling and performance: domain decomposition

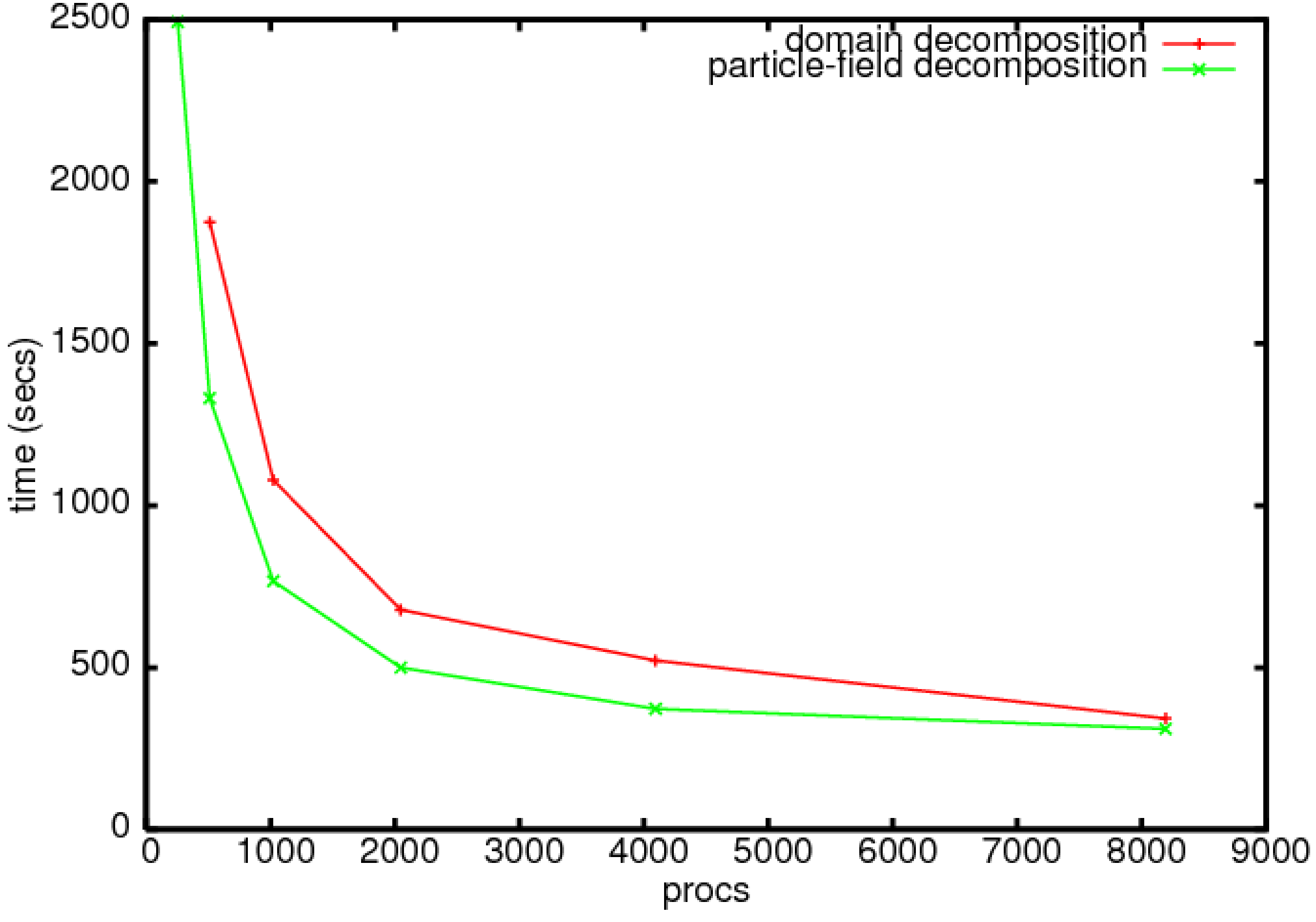


Scaling and performance: particle and field decomposition



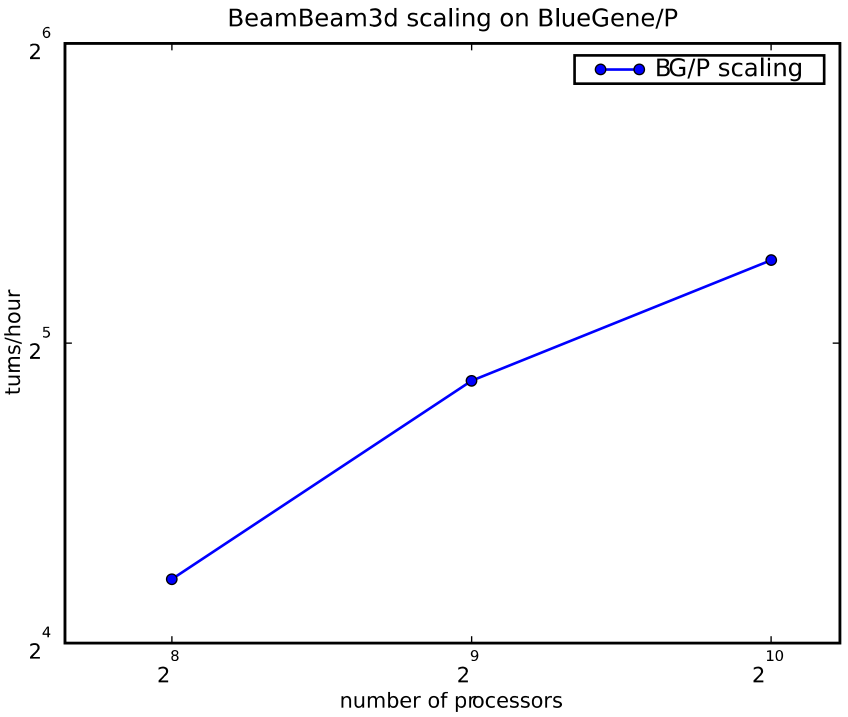
Scaling and performance: decomposition scheme comparison

Strong scaling study on Cray XT



Scaling and performance

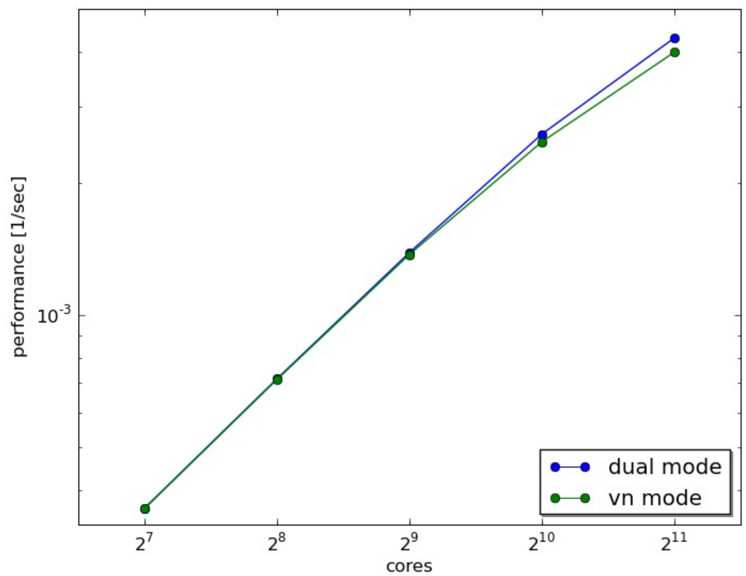
- Parallel scaling of BeamBeam3D on ALCF's Intrepid
- Some simulations require many time steps, but can be utilize “small” grids (O(10^6) degrees of freedom)
  - Example:BeamBeam simulation
    - 800 hrs on Intrepid to simulate 1 sec in Tevatron
    - Effect of interest develops over 15 min
  - Simple solver improvements will not increase scalability by orders of magnitude
    - Not enough degrees of freedom



- Algorithmic improvements are necessary

Scaling and performance, continued

- Strong scaling results from Synergia on Surveyor (ALCF)
  - 64x64x1024 grid, 200M particles



- Weak scaling results from IMPACT-T on Franklin (NERSC)

# processors	time (sec)	mesh size	macroparticles (billions)	efficiency
1000	307.5	64x128x128	1.25	1.0
2000	308.7	64x128x256	2.5	0.996
4000	316.4	64x256x256	5	0.972
8000	320.8	64x256x512	10	0.958
16000	346.6	64x256x1024	20	0.887

Capability development: resistive wall

- Developed for BeamBeam3D simulations of Tevatron
- Dipole component of resistive-wall wakefields
- Includes true multiple bunch implementation in Synergia2
  - Bunches are coupled only through resistive wall
- Kicks are applied to each particle from all earlier slices

$$\frac{\Delta \vec{p}_\perp}{p} = \frac{2}{\pi b^3} \sqrt{\frac{4\pi\epsilon_0 c}{\sigma}} \frac{N_j r_p < \vec{r}_j >}{\beta\gamma} \frac{L}{\sqrt{z_{ij}}}$$

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Capability development: electron cloud

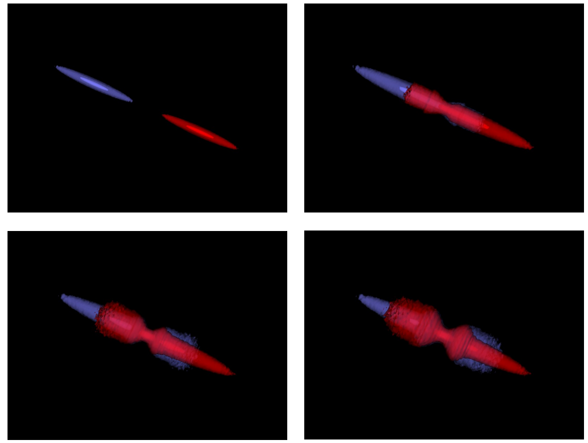
- Electron cloud module under development
  - Electron production
    - TxPhysics
  - Cloud evolution
    - Single-particle transport currently being benchmarked against Vorpal
  - Beam-cloud interaction
    - Sphyraena solver
  - Preliminary componentization completed
- Development paused in order to devote resources to current priorities
  - See Applications

Applications

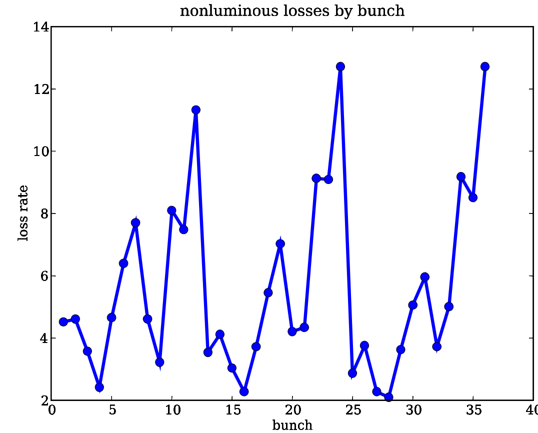
- From the proposal
  - Run II
    - Tevatron
  - ILC
    - Ring To Main Linac (RTML)
    - Damping Ring
      - Dropped due to shift in community priorities
- New priorities
  - Project X
    - Main Injector
    - Debuncher (Mu2e)

Applications: Tevatron

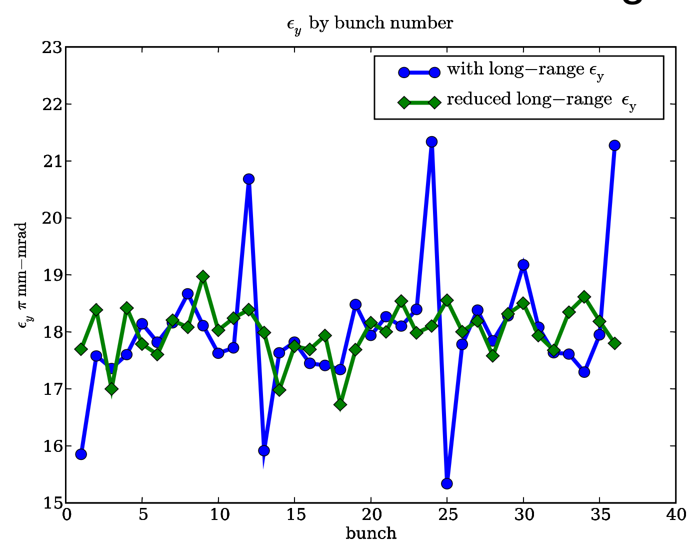
- Multi-physics simulations
  - Beam-beam
  - Resistive Wall
  - Chromaticity
- Large problem: 36x36 bunches
- Run at NERSC and ALCF
  - Stability a problem at NERSC
  - ALCF working well



data

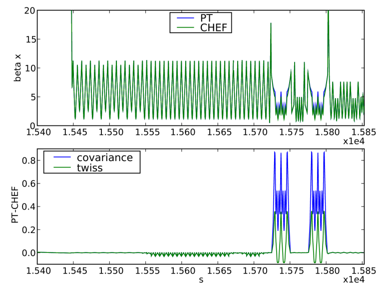


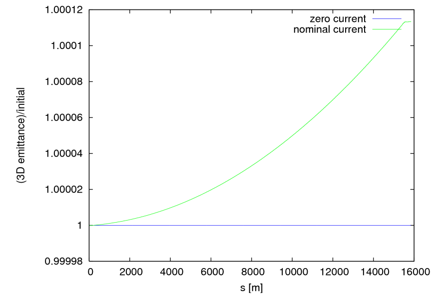
Simulation with and without mitigation

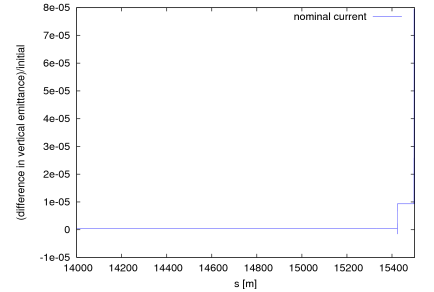


Applications: ILC

- Space charge in the return to main linac (RTML) line was a pressing question in ILC design
- Performed simulations with Synergia2
  - Significant effort in reproducing optics parameters
  - Final report presented to ILC designers
    - Space charge not a show-stopper







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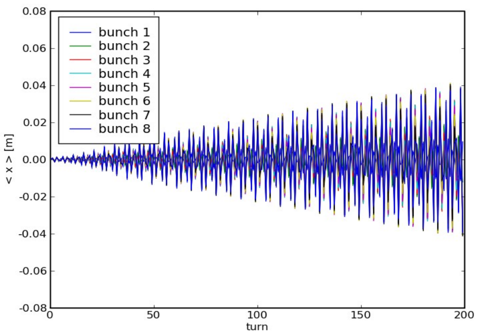
Applications: Project X

- With the sudden cuts in ILC funding, Project X has become a main priority for ComPASS
  - Main Injector
  - Debuncher
- The accelerator physics challenges of the intensity frontier are exactly those that the ComPASS applications are designed to address
  - Multi-physics
    - Space charge
    - Resistive Wall
    - Electron cloud
  - Multi-scale
    - Size: beam size vs. magnet/pipe size, etc.
    - Time: accelerator cycle vs. cloud growth vs. microwave propagation, etc.

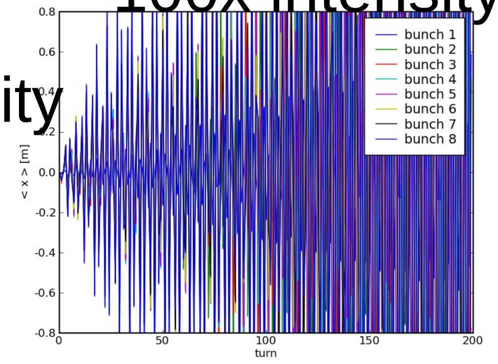
Applications: Main Injector resistive wall

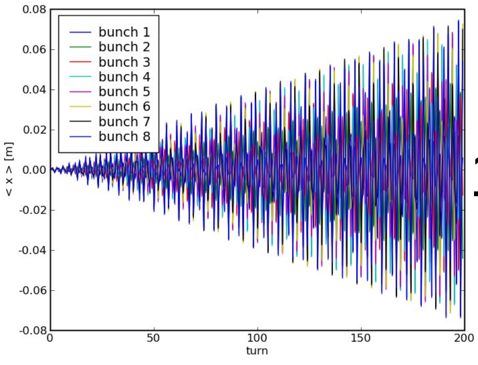
- Testing ground for new resistive wall module
- Well-known issue in Main Injector



nominal intensity

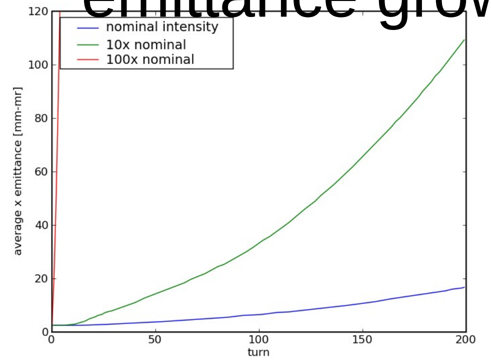
100x intensity





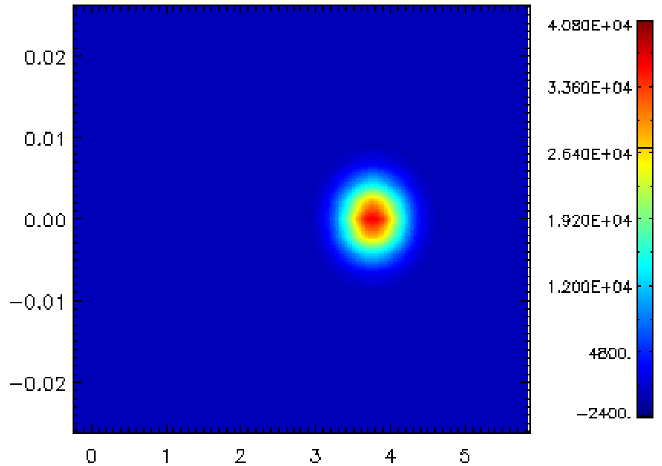
10x intensity

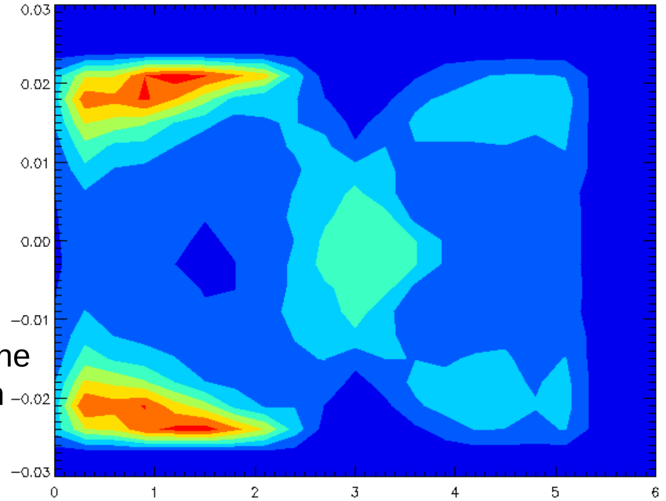
emittance growth



Applications: Microwave electron cloud detector in the Main Injector

- New request
  - Simulate microwave propagation (electron cloud detector apparatus) in the Main Injector
  - Multi-scale and Multi-physics problem well-suited to VORPAL
  - Fermilab-TechX collaboration





Pictures from Vorpal showing an instant snap-shot of the electron cloud multipacting process. X along the beam axis. Y is the vertical axis. Top: the current density along the x axis, and corresponds to a 8 GeV, 5×10^{11} protons bunch, with a Gaussian profile in all 3 direction. Bottom: density/color map of the electrons, on the X-Y plane.

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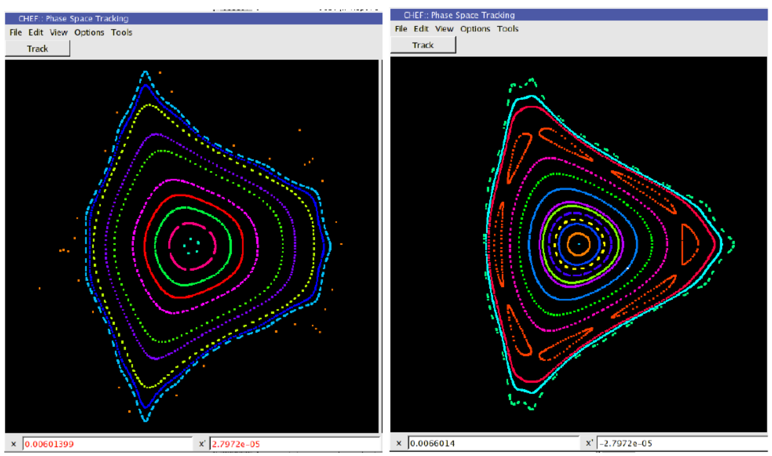
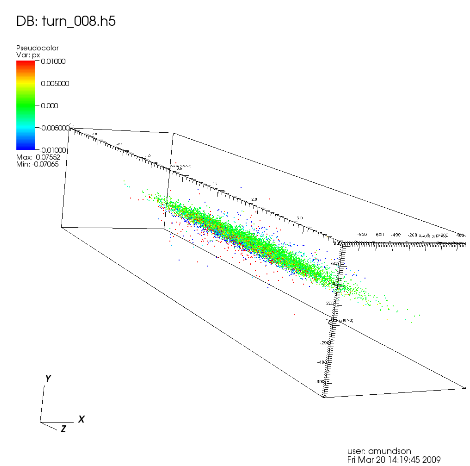
Applications: Debuncher (Mu2e)

- Mu2e project requires switching Debuncher from low-intensity antiproton beam to high-intensity proton beam (10^5 intensity increase)
- Proposed resonant extraction requires highly-nonlinear lattice



Stroboscopic plots of nonlinear lattice



VisIt visualization of bunch at beginning
Of resonant extraction

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